

## Patch Dynamics for Multiscale Problems

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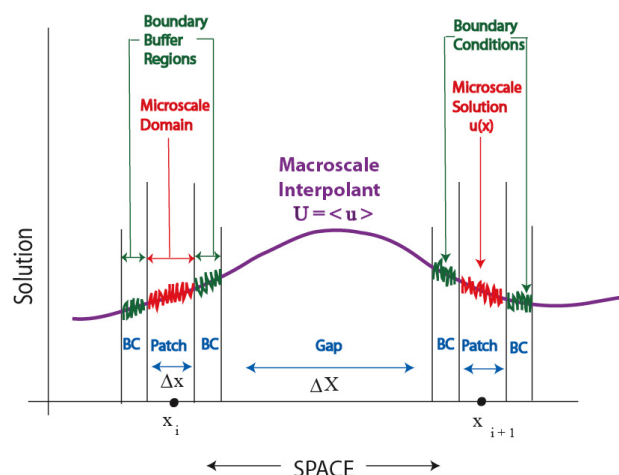
Patch dynamics bridges multiple scales in problems to provide new tools for scientists and engineers to predict the macroscale dynamics of the long time and space scale dynamics using only microscopic simulations over small patches. First developed by Yannis Kevrekidis and his collaborators [1,2], patch dynamics is an efficient approach for bridging these scales. Essentially, hybrid-patch dynamics uses locally averaged properties of short spacetime scales to advance and predict long spacetime scale dynamics.

Most continuum models of reaction and transport processes are derived as conservation laws (mass, species, momentum, and energy) whose average properties are described by partial differential equations (PDEs). However, for a growing class of simulations, including crack propagation, molecular dynamics, Boltzmann kinetic theory models, and modeling the membrane of a living cell where the microscale models are not based on PDEs, but on other physically motivated models. The mechanical properties of deforming materials, such as modeling a materials stress and hardening or predicting defect dynamics as a function of load, often hinge on microscopic transitions that macroscopic-averaged PDE models don't accurately account for.

If we need to predict a systems behavior for macroscopic spacetime scales when only the microscopic model is available, the computational cost can be prohibitive, and will be for the foreseeable future. In situations in which we know a physical processs microscopic description, patch dynamics can help us compute the microscale dynamics on a grid of small patches, which in turn can help us predict the macroscale behavior. Patch dynamics circumvents the need for a closed-form macroscopic description of the system and bypasses the need to explicitly define macroscopic equations, but it still delivers

macroscopic-level information.

There are physical systems where the macroscale equations are unavailable because the microscale dynamics (such as propagation at the tip of a crack) is a highly nonlinear function of small-scale physics, and continuum models can't capture this singular behavior. In other physical models, the macroscopic equations for average quantities such as mass, momentum, or energy are known, but the equations for the higher moments of the variables distribution on the microscale are needed, but are not known. Patch dynamics can predict system behavior of these higher moments for long spacetime scales without explicit evolution equations such as PDEs.



*Figure 1. One-dimensional physical system. The microscale variable  $u(x)$  varies rapidly, but the macroscopic variables  $U = (\langle u \rangle, \langle u_x \rangle, \langle u_{xx} \rangle, \text{ and so on})$  vary slowly. The boundary conditions for the patches are defined by extending the microscale solution into a buffer region surrounding each patch. The patches communicate with each other via boundary conditions similar to the way finite difference approximations of partial differential equations communicate to the surrounding grid points.*

Finite difference and finite element methods are standard indispensable algorithms for solv-

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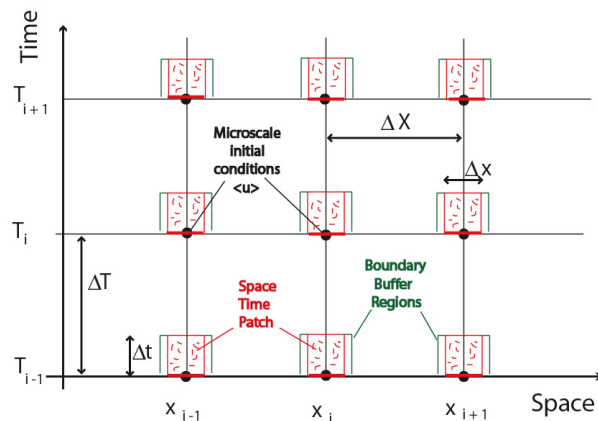


Figure 2. Space-time plot for the patches in Figure 1. The microscale solution is advanced in small space-time patches until accurate approximations of the time derivatives of the macroscale variables  $U$  can be obtained over the space-time patch. These time derivatives are used to advance the macroscale variables a macroscale time step, and the process repeats.

ing PDEs in science and engineering. The tools and analysis in applying these methods have a lot in common with patch dynamics. In patch dynamics, as well as in finite difference and element methods, we first define a mesh to cover the domain of interest. Next, we define the macroscale solution  $U$  at the grid points and approximate the PDEs with finite differences to define the time derivative  $U_t$  at the grid points.

The finite difference method is an ingenious technique that uses a PDE to combine the neighboring values of the solution on a grid to define a time derivative for the solution at the grid points. These time derivatives advance the solution in time by using a numerical integration method, such as a Runge-Kutta method. We determine the approach's accuracy by how well the mesh resolves the underlying solution, how accurately the PDEs finite difference approximation defines  $U_t$ , and how accurately the numerical integration method advances the solution in time.

As in a finite difference method, the first step in patch dynamics is to define an appropriate grid that resolves the macroscale structure as in Figure 1. In finite difference methods, we solve for the value of the averaged microscale at each of the grid points. In patch dynamics, the grid points are stretched into the small patches (regions) where the microscopic model will be solved. Next, we generate microscopic initial conditions in the patch to agree with the macroscale averages at the grid points. The global macroscopic solution is defined by interpolating the macroscale averages at the grid points. This interpolant defines the microscale boundary conditions at the edges of the patches and provides communication across the spatial gaps between the patches. The microscale solution is then advanced a short time in each patch using the microscopic model, as shown in Figure 2. The integration of microscopic model creates changes in the macroscale averages over the patch. These changes define the time derivatives of averaged quantities and their moments. As in the PDE case, these time derivatives are used to advance the macroscopic variables in time via a numerical integration method.

## Acknowledgements

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## References

- [1] J. M. Hyman, J. M., *Patch Dynamics for Multiscale Problems*, Computing in Science and Engineering, Vol. 7, No. 3, 2005, 47-53
- [2] Kevrekidis, I. G., C.W. Gear, J.M. Hyman, P.G. Kevrekidis, O. Runborg, C. Theodoropoulos, *Equation-Free Coarse Grained Multiscale Computation: Enabling Microscopic Simulators to Perform Systems-Level Tasks*, Comm. in the Math. Sciences, 14, 715-762, 2003